

Claims

1. Method for information storage and data processing comprising the step of thermo inducing or  
5 photo inducing double-bond shifts (DBS) in substituted [4n]-annulenes, thus generating transitions between two different conjugation states with at least one substituent.

10 2. Method according to claim 1, whereby the two different conjugation states are the conjugation on-state and conjugation off-state of the annulene core  $\pi$ -electrons relative to the substituent  $\pi$ -electrons.

15 3. Method according to claim 1 or 2, whereby said [4n]-annulenes are bicyclic [4n]-annulenes.

20 4. Method according to claim 3, whereby said bicyclic [4n]-annulenes are heptalenes.

5. Method according to any of the claims 1 to 4, whereby the [4n]-annulenes are substituted by at least one group comprising an extended conjugated  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system  
25 of the [4n]-annulene core.

6. Method according to claim 5, whereby the [4n]-annulenes are substituted in 1,2- or 1,4-position relative to each other by two groups having an extended  
30 and conjugated  $\pi$ -electron system.

7. Method according to any of the preceeding claims, whereby a multitude of [4n]-annulene molecules are arranged in a 1-dimensional or in a 2-dimensional or  
35 in a 3-dimensional way and wherein said conjugation states are spatially non-uniformly modulated.

8. Method according to claim 7, whereby a conformationally restricted matrix system is generated by modulating said conjugation states.

5                   9. Method according to any of the preceeding claims, whereby the [4n]-annulene molecules are embedded in a matrix.

10                   10. Method according to claim 9, wherein the matrix comprises a low-melting glass or polycarbonates, polyacetates, methacrylates, styrenes and copolymers thereof, as well as copolymers with polymerisable [4n]-annulenes.

15                   11. Method according to any of the claims 7 - 10, whereby a holographic grating is generated by modulating said conjugation states.

20                   12. Method according to one of the claims 7 to 11, wherein the spacially non-uniformly modulated conjugation states are generated by a low-energy laser that provides for a local heating so bring the [4n]-annulenes into switching condition and whereby the laser light causes locally, if required, the switch from the  
25 conjugative on-state to the conjugative off-state.

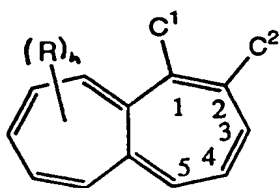
30                   13. Method according to any of the claims 6-12, comprising further to said step of modulating a multitude of [4n]-annulene molecules in a 1-dimensional or 2-dimensional or 3-dimensional way and wherein said conjugation states are spacially non-uniformly modulated, a further step wherein at least one of the optical, electrical or magnetic properties being attributable to said switchable conjugation states is determined and pro-  
35 cessed.

14. Method according to any of the preceeding claims, wherein said conjugation states are determined by an optical read-out step.

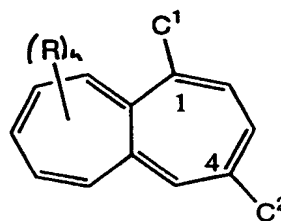
15. Method according to any of the preceeding claims, wherein the determination of the spacially non-uniformly modulated conjugation states is used for the optical reading of information.

16. Method according to any of the preceeding claims, wherein the determination of the spacially non-uniformly modulated conjugation states is used for optical switching and computing.

17. Substituted [4n]-heptalenes of the general formula (I) or (II) being optically and/or thermally switchable, based on thermal or photochemical double-bond shifts (DBS),



(I)



(II)

whereby  $C^1$  and  $C^2$  represent independently from each other a hydrogen atom, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkoxy group, a substituted or unsubstituted aryl- $C_1$ - $C_{12}$ -alkyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkenyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -conjugated alkenyl group, a substituted or unsubstituted  $C_1$ - $C_{12}$ -alkinyl group, a substituted or an unsubstituted phenyl group, a substituted or an unsubstituted heterocyclic group, a cyano group, a nitro group, a thiocyanate group, a  $C_1$ - $C_{12}$ -ester group being optionally polymerisable with copolymers, with the proviso that at least one of

said substituents  $C^1$  and  $C^2$  contains a  $\pi$ -electron system which is in conjugation with the  $\pi$ -electron system of the heptalene core, and

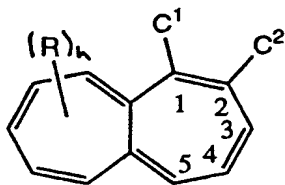
whereby said  $[4n]$ -heptalenes can comprise at least one further substituent R being selected from the above indicated groups with n being 0-8,

provided that if one of the at least one further substituents R is a isopropyl group at the position 9 of the heptalene ring, the substituent at the position 6 must not be a methyl group.

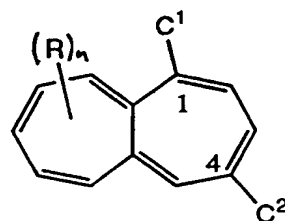
18.  $[4n]$ -heptalenes according to claim 17, whereby,  $C^1$  and  $C^2$  represent independently from each other a hydrogen atom, a methyl group, a phenyl group, an ethyl ester group, a methyl ester group, a (E)-PhCH=CH group, a (E)-4-MeOC<sub>6</sub>H<sub>4</sub>CH=CH group, a (E)-4-ClC<sub>6</sub>H<sub>4</sub>CH=CH group, a 4-MeOC<sub>6</sub>H<sub>4</sub> group, a -CH=CH-CH=CH-C<sub>6</sub>H<sub>5</sub> group, a -CH=CH-C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>-4 group, a -CH=CH-C<sub>6</sub>H<sub>4</sub>OMe-4 group

19.  $[4n]$ -heptalenes according to claim 17 or 18, whereby said further substituents R are selected from the group comprising substituted or unsubstituted C<sub>1</sub>-C<sub>12</sub>-alkyl groups or photoactive diazo-containing groups, like azobenzen.

20. Method for the preparation of substituted heptalenes of the formula (I) or (II),



(I)



(II)

whereby  $C^1$ ,  $C^2$ , R and n are as above defined, comprising the steps of

(a) obtaining a heptalene-dicarboxylate by a reaction of a correspondingly substituted azulene with acetylenedicarboxylate,

(b) transforming said methyl substituent at  
5 the position 1 of the heptalene ring into the desired conjugated substituent having an extended  $\pi$ -electron system.

21. Method according to claim 20, whereby a  
10 heptalene-4,5-dicarboxylate carrying a methyl substituent at the position 1 of the heptalene ring is obtained.

22. Method according to claim 20 or 21,  
further comprising a step (c) wherein at least one of the  
15 carboxylate groups within the heptalene ring is replaced by a conjugated substituent containing an extended  $\pi$ -electron system.

23. Method according to claim 22, wherein the  
20 carboxylate group at the position 4 of the heptalene ring is replaced by a conjugated substituent containing an extended  $\pi$ -electron system.

24. An optical storage device comprising at  
25 least one substituted [4n]-annulene according to one of the claims 17-19.

25. A non-linear optical device comprising at  
least one substituted [4n]-annulene according to to one  
30 of the claims 17-19.

26. Use of substituted [4n]-annulenes undergoing thermally induced or photo-induced double-bond shifts (DBS) thus generating two different conjugation  
35 states with at least one substituent, for information storage and data processing.